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RELATIVE RESONANCE LINE STRENGTHS IN THE NEON I AND ARGON I ISOELECTRONIC* SEQUENCES

by

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ABSTRACT

We have calculated relative line strengths for the resonance lines of ions in the Neon I isoelectronic sequence through Iron XVII, and in the Argon I sequence through Iron IX. We used intermediate coupling theory, and evaluated the necessary parameters using observed energy levels. The relative line strength results for the Neon I sequence agree well with previous calculations using Hartree-Fock wavefunctions. For Iron IX, whose resonance lines are observed in the solar UV spectrum, we calculated absolute line strengths, oscillator strengths, and transition probabilities using the scaled Thomas-Fermi potential to obtain the radial transition integral. The transition probabilities obtained are: $\lambda 103.58$, $A = 4.6 \times 10^{10}$ sec^{-1} ; $\lambda 105.24$, $A = 2.7 \times 10^{10}$ sec^{-1} .

I. INTRODUCTION

The resonance lines of Iron XVII (in the Neon I isoelectronic sequence) and Iron IX (in the Argon I sequence) have been identified in the solar UV spectrum (Jordan 1965). Garstang (1966b) and Kastner, Omidvar and Underwood (1967) have calculated the oscillator strengths of the Iron XVII lines (16.774Å and 17.051Å), as an aid in the interpretation of their observed intensities. Both calculations were based in part on the intermediate coupling (IC) approximation (Condon and Shortley 1951).

We have calculated the oscillator strengths and transition probabilities of the Iron IX resonance lines (103.58Å and 105.24Å) using a modification of Garstang's method. We have also calculated the relative strengths of the resonance lines of all ions in the Argon I sequence preceding Iron IX, and for most of the Neon I sequence through Iron XVII. Our results for the Neon I sequence agree well with those of Kastner et al. (1967).

II. RARE-GAS RESONANCE LINE STRENGTHS IN INTERMEDIATE COUPLING

The resonance lines in rare gas-like ions arise from the transitions $np^6\ {}^1S_0 - np^5n's\ {}^1P_1$ and $np^6\ {}^1S_0 - np^5n's\ {}^3P_1$. The spin-orbit interaction intermixes the two $J = 1$ wavefunctions of the $np^5n's$ configuration; this explains the existence of a nonzero dipole moment for the second transition, which is forbidden in pure LS-coupling.

In intermediate coupling theory, the energies of the four levels arising from the p^5s configuration are given by the eigenvalues of the energy matrix shown in Figure 1 (Garstang 1966a).

/Figure 1 Here/

Three parameters are involved: the Slater integrals F_0 and G_1, and the spin-orbit integral ζ_{np}. The eigenvectors of the energy matrix represent the wavefunctions: the $J = 1$ eigenvectors have the general form

$$\Psi_- = \alpha|^1P_1\rangle + \beta|^3P_1\rangle \qquad (1)$$

$$\Psi_+ = -\beta|^1P_1\rangle + \alpha|^3P_1\rangle \quad . \qquad (2)$$

The corresponding eigenvalues are

$$\lambda_\pm = -F_0 + \zeta/4 \pm \sqrt{((G_1-\zeta/4)^2 + \zeta^2/2)} \quad . \qquad (3)$$

The ratio of the resonance line strengths, defined as

$$r = \frac{|\langle^1S_0|P|\Psi_-\rangle|^2}{|\langle^1S_0|P|\Psi_+\rangle|^2} \quad , \qquad (4)$$

is just

$$r = \alpha^2/\beta^2 \quad . \qquad (5)$$

The strength of the $p^6\ {}^1S_0 - p^5 s\ {}^1P_1$ transition in pure LS-coupling can be obtained from the tables of Shore and Menzel (1965): it is $6\sigma^2$, where σ^2 is the usual radial transition integral. Thus the strengths of the two resonance lines are

$$S({}^1S_0 - \Psi_+) = 6\sigma^2/(1+r) = 6\sigma^2\beta^2 \qquad (6)$$

and

$$S({}^1S_0 - \Psi_-) = 6\sigma^2 r/(1+r) = 6\sigma^2\alpha^2 \quad . \qquad (7)$$

The usual procedure in the calculation of these line strengths in intermediate coupling is to determine F_0, G_1, and ζ_{np}, evaluate the energy matrix, determine the $J = 1$ eigenvectors to obtain α and β, and then use equations (6) and (7). (See, e.g., Garstang 1966b).

Instead, we have evaluated α and β directly in terms of G_1 and ζ_{np}, and then used equation (5) to obtain

$$r = \frac{(9\mu^2-8\mu+16)^{1/2} + (\mu-4)}{(9\mu^2-8\mu+16)^{1/2} - (\mu-4)} \quad , \qquad (8)$$

where $\mu \equiv \zeta_{np} / G_1$. (The appearance of the constant term $-F_0$ in each diagonal element of the energy matrix, and nowhere else, means that the eigenvectors are independent of F_0.) Thus we need only determine ζ_{np} and G_1 to obtain r , using equation (8). Figure 2 illustrates the behavior of r as μ goes from 0 (pure LS-coupling) to ∞ (pure jj-coupling).

/Figure 2 Here/

III. DETERMINATION OF THE INTERMEDIATE COUPLING PARAMETERS

We discuss three methods of determining the values of the Slater and spin-orbit integrals for a p^5s configuration.

The first method is applicable when the energies of all four levels of the configuration are known. In this case F_0 , G_1 and ζ_{np} can be chosen so that the eigenvalues of the p^5s energy matrix give a least-squares fit to the observed energies. (See, e.g., Garstang and Van Blerkom 1965). Configuration interaction, if it is present, generally perturbs the energies enough that a poor fit results, so that this method provides an indication of the validity of the IC approximation.

The second method makes use of the observation of Condon and Shortley (1951, p. 308) that the spin-orbit integral ζ_{np} for the np^5 core in the rare gases can be obtained from the ground-state doublet splitting in the parent ion, which is $3\zeta_{np} / 2$. (For example, the ground state splitting in

Argon II is 1432 cm^{-1}, which gives $\zeta_{3p} = 954.67\ cm^{-1}$: the average value of ζ_{3p} obtained in least-squares fits of the configuration 4s, 5s, 6s, and 7s in Argon I is 943.05.) In treating Iron XVII, Garstang (1966b) used the Iron XVIII splitting (obtained by extrapolation) to get ζ_{2p}, and determined F_0 and G_1 by forcing a fit to the two known $2p^5 3s$ energy levels in Iron XVII (Moore, 1952). Note that there is only just enough data to make the calculations possible: no measure of the correctness of the IC approximation can be obtained with this method.

A third method is that of Kastner et al. (1967), who treated the Neon I sequence from Sodium II to Iron XVII. They calculated values of F_0, G_1, and ζ_{2p} for each member of this sequence directly from Hartree-Fock wavefunctions generated by the computer program of Froese (1963).

We have treated the Argon I sequence through Iron IX, using the least-squares method for the first three members. For the rest of the sequence we obtained ζ_{3p} from the ground-state splitting of the parent ions, as Garstang did. But since the only additional parameter needed was G_1, we obtained it from the difference of the $J = 1$ energy levels tabulated by Moore (1949, 1952): if we designate this difference by d, we obtain from equation (3)

$$G_1 = (\zeta_{np}/4) \pm \sqrt{((d/2)^2 - \zeta_{np}^2/2)} \quad . \qquad (9)$$

The positive sign in equation (9) holds for the Argon I sequence at least as far as Iron IX: it gives values of G_1 which agree with those obtained from least-squares fits for the first three members of the sequence, and which vary smoothly with Z. Our results are given in Table 1.

In Table 2, we give the results of our calculations of line strength ratios for the Neon I sequence, and the results of Kastner et al. (1967) for comparison. We have used the extrapolation of Rohrlich and Pecker (1963) to obtain the parent ion ground-state splittings. The agreement is quite good, except as noted below. This good agreement reflects favorably on the Hartree-Fock calculations, inasmuch as our method is based directly on observable quantities.

In applying equation (9) to Ti XIII, V XIV, Cr XV, and Mn XVI, we obtained negative values for the quantity $(d/2)^2 - \zeta_{2p}{}^2/2$, so that our method fails in these cases. An extrapolated plot of μ vs Z indicates that $\mu \approx 4$ for Vanadium XIV: equation (9) shows that for $\mu \approx 4$, $(d/2)^2 - \zeta^2/2$ will be small, but in theory should be positive. However, this quantity is a difference of two large numbers, each subject to error, so that negative values are not surprising. The relatively poor agreement of our result for Scandium XII with that of Kastner et al. is probably due to this feature of our method, since in this case $\mu = 3.80$. In the Argon I sequence, however, the largest value of μ is 2.39 (for Iron IX), so that our method should work well.

The radial transition integral σ^2 for the Iron IX resonance lines was calculated using a modification by J. Cooper (unpublished) of the computer program of Stewart and Rotenberg (1965). The result was $\sigma^2 = 0.020$.

We then calculated the line strengths, using equations (6) and (7) and the value of r given in Table 1. Table 3 gives the line strengths, oscillator strengths, and transition probabilities for these lines.

IV. SUMMARY AND COMMENTS

The Iron IX transition probabilities given here should be of use in the determination of the conditions under which the lines are limitted from the solar corona. Calculations of cross-sections for excitation of the Iron IX ion by electron impact are needed to complement our results.

Kastner et al. (1967) have observed that the ratio of intensities of the two solar UV lines tentatively identified as arising from Magnesium III is much higher than the corresponding ratio of the line strengths. They suggest that configuration interaction in Magnesium III may be responsible for the discrepancy. However, we found that the IC theory gave energy levels for the $2p^5 3s$ configuration of Mg III in excellent agreement with those observed: the rms deviation was $0.207\ cm^{-1}$. We conclude that the calculated line strength ratio is correct, and that the identification of the solar lines is probably incorrect.

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REFERENCES

Condon, E. U. and Shortley, G. H. 1951, The Theory of Atomic Spectra, (Cambridge: At the University Press), Chap. XI.

Froese, C. 1963, Canadian J. Phys. 41, 1895-1910.

Garstang, R. H. 1966a, J.I.L.A. Rept. No. 85, (Joint Institute for Laboratory Astrophysics, Boulder, Colorado).

- 1966b, Pub. Astron. Soc. Pacific, 78, 399-406.

Garstang, R. H. and Van Blerkom, J. 1965, J. Opt. Soc. Am. 55, 1054-1057.

Jordan, C. 1965, Communs. Univ. London Obs., No. 68.

Kastner, S. O., Omidvar, K., and Underwood, J. H. 1967, Ap. J. 148, 269-273.

Moore, C. E. 1949, Atomic Energy Levels, N.B.S. Circ. 467 (Washington, D.C.), Vol. I.

- 1952, ibid., Vol. II.

Rohrlich, F. and Pecker, C. 1963, Ap. J. 138, 1246-1261.

Shore, B. W. and Menzel, D. H. 1965, Ap. J. Suppl. Series, Vol. XII, 187-214.

Stewart, J. C. and Rotenberg, M. 1965, Phys. Rev. 140A, A1508-A1519.

TABLE 1

RATIOS OF RESONANCE LINE STRENGTHS IN THE ARGON I SEQUENCE

Ion	Resonance Line Wavelengths (Å, vac)		ζ_{3p} (cm^{-1})	G_1 (cm^{-1})	r
ArI	1066.66	1048.22	939.19	725.31	0.255
KII*	612.61	600.74	1878.93	1134.33	.382
CaIII	409.96	403.72	2040.03	1728.06	.216
ScIV	298.43	293.25	2885.	2866.	.160
TiV	228.90	225.34	3893.	3053.	.248
VVI	182.05	179.32	5107.	3372.	.332
CrVII	148.74	146.53	6600.	3592.	.445
MnVIII	124.05	122.17	8353.	3973.	.534
FeIX	105.24	103.58	10455	4375.	0.624

*Least-squares fit to energy levels indicates presence of configuration interaction in $3p^5 4s$ configuration of this ion.

TABLE 2

RATIOS OF RESONANCE LINE STRENGTHS IN THE NEON I SEQUENCE

Ion	Resonance Line Wavelengths (Å, VAC)		ζ_{2p} (cm^{-1})	G_1 (cm^{-1})	r	r (kou)*
NeI	743.71	735.88	517.82	743.46	0.076	-
NaII	376.37	372.07	904.91	1623.34	0.048	0.049
MgIII	234.26	231.73	1474.70	2453.22	0.056	0.053
AlIV	161.69	160.07	2196.98	3274.69	0.070	0.076
SiV	118.97	117.86	3400.	3984.	0.115	0.112
PVI	91.47	90.65	4845.	4812.	0.160	0.157
SVII	72.66	72.03	6753.	5411.	0.238	0.214
ClVIII	59.19	58.67	9067.	6071.	0.324	0.296
AIX	49.18	48.73	12042.	6957.	0.408	0.375
KX	41.54	41.15	15650.	7041.	0.572	0.505
CaXI	35.58	35.21	20019.	8147.	0.644	0.606
ScXII	30.82	30.48	25239.	6642.	0.97†	0.72
FeXVII	17.05	16.77	68033.	11689.	1.25	1.19

*Kastner, Omidvar and Underwood (1967).

†See §3 for comment on accuracy of this result.

TABLE 3

ABSOLUTE STRENGTHS OF IRON IX RESONANCE LINES

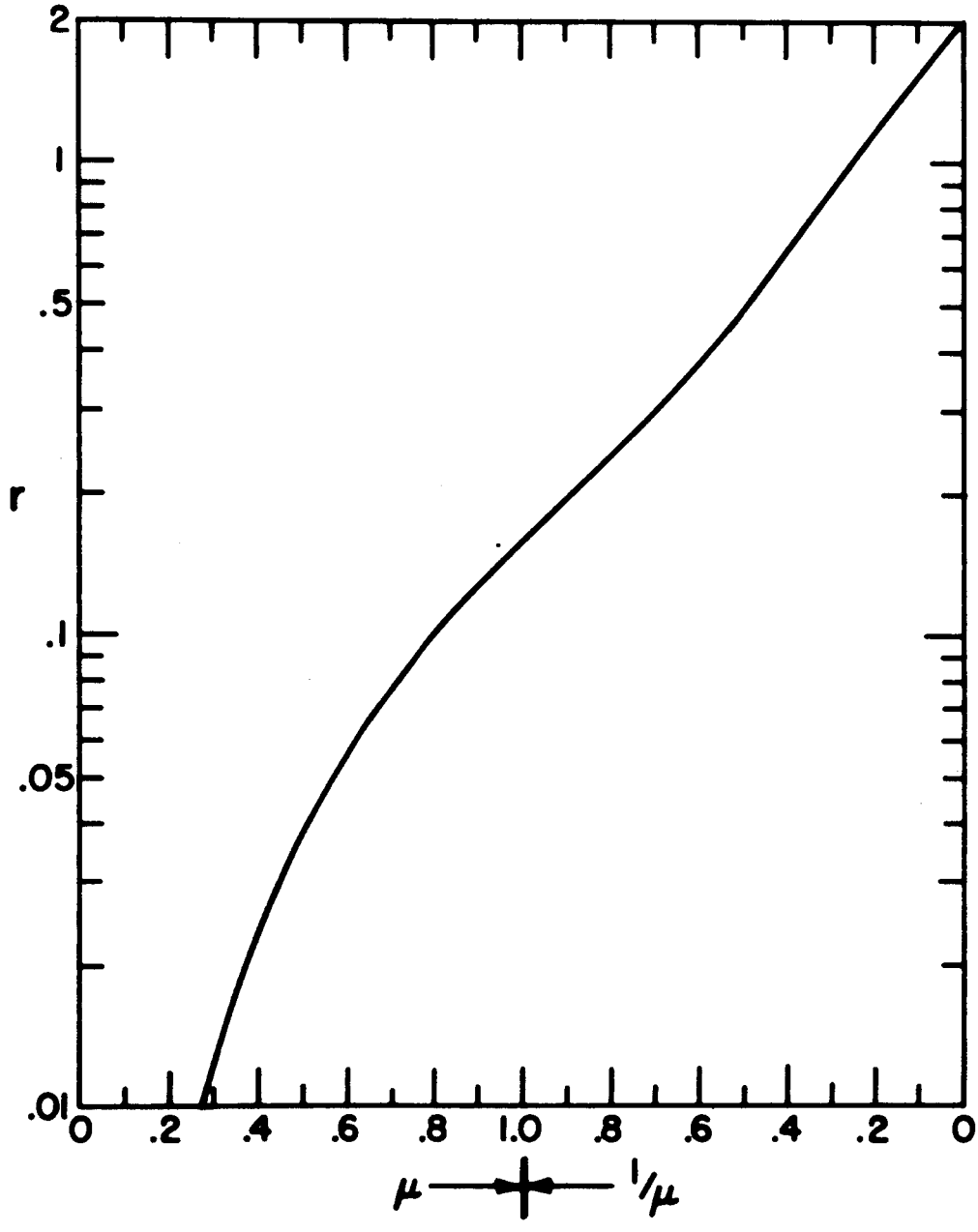
Wavelength (Å, vacuum)	S (at. u.)	f_{ik}	A_{ki} (sec^{-1})
103.58	.075	.22	4.6×10^{10}
105.24	.047	.14	2.7×10^{10}

Fig. 1. -- Energy matrices for the p^5s configuration.

$$-F_0 +$$

$^3P_0$	$-G + \zeta_{np}$	0	0	0
$^1P_1$	0	G_1	$\zeta_{np}/\sqrt{2}$	0
$^3P_1$	0	$\zeta_{np}/\sqrt{2}$	$-G_1 + \zeta_{np}/2$	0
$^3P_2$	0	0	0	$-G_1 - \zeta_{np}/2$

Fig. 2. -- Resonance line strength ratio r in rare gas-like ions, throughout intermediate coupling, as a function of $\mu = \zeta/G_1$.


2
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